UPM Activities on the STLs processing (Task 6.2) and the generation of DPA cross section library up to 150 MeV (Task 4.1)

Oscar CABELLOS and Emilio CASTRO

Universidad Politécnica de Madrid (UPM)

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UPM Activities in F4E-GRT-168.1: "Nuclear Data Improvements & Development of tools - Nuclear Data Evaluation"

Task 4.1 : Generation of a complete damage energy and dpa cross section library up to 150 MeV based on JEFF-3.1.1 and suitable approximations (UPM)

Sub-tasks:

(1) JEFF damage energy analysis
(2) Approximations above 20 MeV
(3) Processing of data library up to 150 MeV (the present library is limited to 20 MeV)

Task 6.2 : Postprocessing of photonuclear libraries (**by CCFE**) and thermal scattering tables (**by UPM**) at the backend of the calculational system (CCFE/UPM)

Sub-tasks on Photonuclear or STLs libraries:

(1) Revision of evaluated nuclear data
(2) Processing and testing
(3) Release

In May 2012, CCFE proposed to work on photonuclear libraries. And, UPM agreed that task responsibilities are interchanged between CCFE (Photonuclear) and UPM (STLs). With no impact on schedule and budget.

UPM Activities in F4E-GRT-168.1: In addition … Education and Training

1. **Master Thesis Project** by Beatriz Cabellos within our Master Programme in Nuclear Science and Technology

   Title: ESTUDIO DE LA GENERACIÓN DE LIBRERÍAS DE DAÑO NEUTRÓNICO UTILIZANDO LIBRERÍAS EVALUADAS DE DATOS NUCLEARES” (**“Study of DPA Libraries Generation Using Evaluated Nuclear Data Libraries”**)

   September 2011

2. **Master Thesis Project** by Azucena Bello within our Master Programme in Energy Engineering

   Title: ESTUDIO DE LIBRERÍAS EVALUADAS FOTONUCLEARES Y PROCESAMIENTO PARA MCNP **(“Study of Photonuclear Evaluated Data Libraries and Processing in ACE Format”**)

   November 2012

3. **Master Thesis Project** by Emilio Castro within our Master Programme in Nuclear Science and Technology

   Title: ESTUDIO DE LIBRERÍAS DE DISPERSIÓN TÉRMICA Y PROCESAMIENTO EN FORMATO ACE” (**“Study of Scattering Thermal Libraries and Processing in ACE Format”**)

   September 2013

Task 4.1 : Damage energy and dpa cross section library : Background

- **Damage energy analysis:** Analysis of the DPA processing above 20 MeV in JEFF-3.1.1
  - Damage Energy Cross Section processed with NJOY
  - This problem was reported to NEA (***Yolanda Rugma***) by Oscar Cabellos in November 2006
  - Also, to F4E (***Leichtle Dieter***) in January 2010

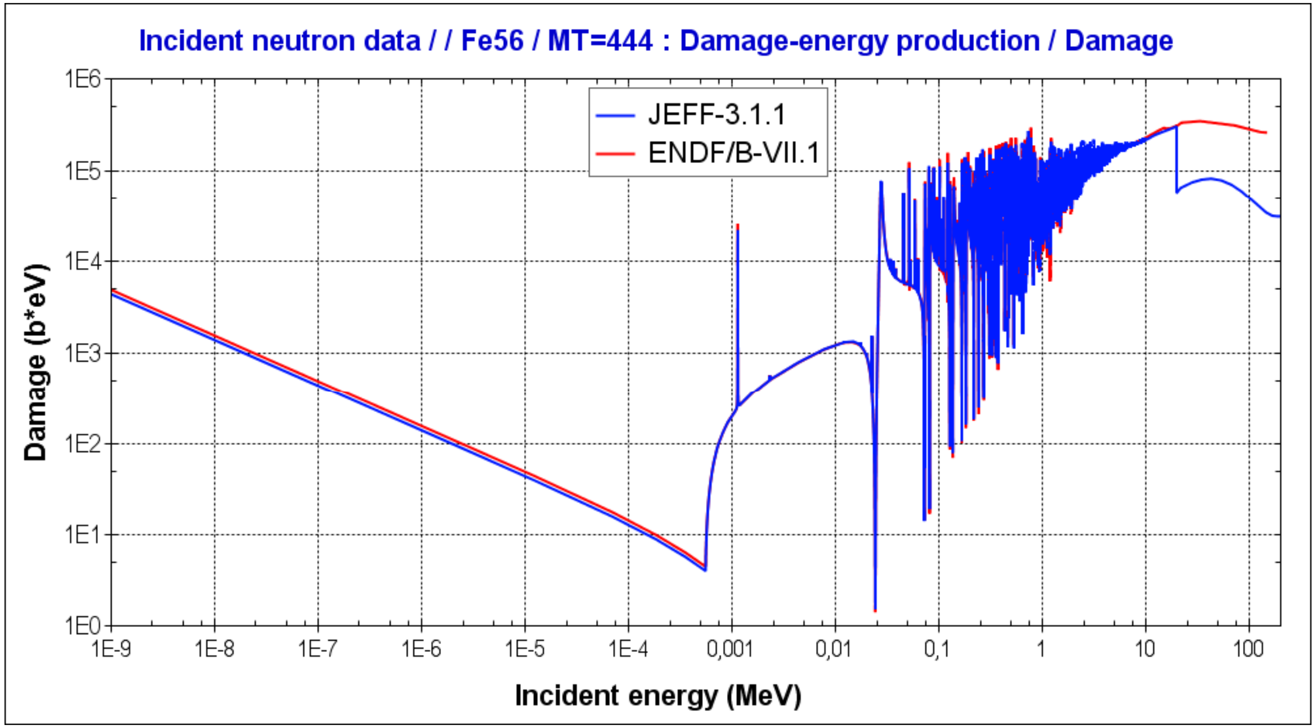


Figure. A comparison of Fe^{56} Damage Energy Cross Section processed with NJOY99.364. JEFF-3.1.1 versus ENDF/B-VII.1

Task 4.1 : Analysis of dpa above 20 MeV

- After some preliminary analysis we concluded: "JEFF-3.1 files (in particular for Fe56) do not have recoil information above 20 MeV" (***private communication by Arjan Koning***)

JEFF3.1

Energy	**damage**	**%damage**	
2,5000E+07	6,8124E+04	0,9878	neutron heating for mt 2 q0 = 0.0000E+00 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 1 q = 0.0000E+00
2,5000E+07	1,7596E+02		file six heating for mt 5, particle = 1001 q = 0.0000E+00
2,5000E+07	5,0585E+01		file six heating for mt 5, particle = 1002 q = 0.0000E+00
2,5000E+07	1,3072E+01		file six heating for mt 5, particle = 1003 q = 0.0000E+00
2,5000E+07	9,8408E-01		file six heating for mt 5, particle = 2003 q = 0.0000E+00
2,5000E+07	5,9711E+02		file six heating for mt 5, particle = 2004 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 0 q = 0.0000E+00
Total	6,8962E+04	1,0000	
TOTAL	**Damage (444)**		
2,5000E+07	**6,8962E+04**		final kerma factors

Figure. Extract of NJOY (HEATR) output Fe56 - JEFF-3.1.1

Task 4.1 : Analysis of dpa above 20 MeV

ENDFB-VI.R8

Energy	**damage**	**%damage**	
2,5000E+07	8,6765E+04	0,2600	neutron heating for mt 2 q0 = 0.0000E+00 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 1 q = 0.0000E+00
2,5000E+07	1,9507E+02		file six heating for mt 5, particle = 1001 q = 0.0000E+00
2,5000E+07	6,0507E+01		file six heating for mt 5, particle = 1002 q = 0.0000E+00
2,5000E+07	6,6042E+00		file six heating for mt 5, particle = 1003 q = 0.0000E+00
2,5000E+07	3,7607E+02		file six heating for mt 5, particle = 2004 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 18037 q = 0.0000E+00
…	…	…	…
2,5000E+07	1,7571E+04	0,0526	file six heating for mt 5, particle = 24052 q = 0.0000E+00
2,5000E+07	1,9213E+03		file six heating for mt 5, particle = 24053 q = 0.0000E+00
2,5000E+07	1,1395E+03		file six heating for mt 5, particle = 24054 q = 0.0000E+00
2,5000E+07	2,4855E+02		file six heating for mt 5, particle = 24055 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 25050 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 25051 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 25052 q = 0.0000E+00
2,5000E+07	1,5863E+02		file six heating for mt 5, particle = 25053 q = 0.0000E+00
2,5000E+07	1,2596E+04	0,0377	file six heating for mt 5, particle = 25054 q = 0.0000E+00
2,5000E+07	6,0763E+04	0,1821	file six heating for mt 5, particle = 25055 q = 0.0000E+00
2,5000E+07	5,2049E+03	0,0156	file six heating for mt 5, particle = 25056 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 26052 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 26053 q = 0.0000E+00
2,5000E+07	7,4113E+03	0,0222	file six heating for mt 5, particle = 26054 q = 0.0000E+00
2,5000E+07	9,5612E+04	0,2865	file six heating for mt 5, particle = 26055 q = 0.0000E+00
2,5000E+07	4,3405E+04	0,1301	file six heating for mt 5, particle = 26056 q = 0.0000E+00
2,5000E+07	0,0000E+00		file six heating for mt 5, particle = 0 q = 0.0000E+00
Total	**3,3374E+05**	1,0000	

Total	**Damage(444)**	
2,5000E+07	**3,3374E+05**	final kerma factors

Figure. Extract of NJOY (HEATR) output Fe56 –ENDF/B-VI.R8

Task 4.1 : Approximations above 20 MeV ?

- Approximation: JEFF-3.1.1 with MT5-MT6 taken from ENDF/B-VII.1

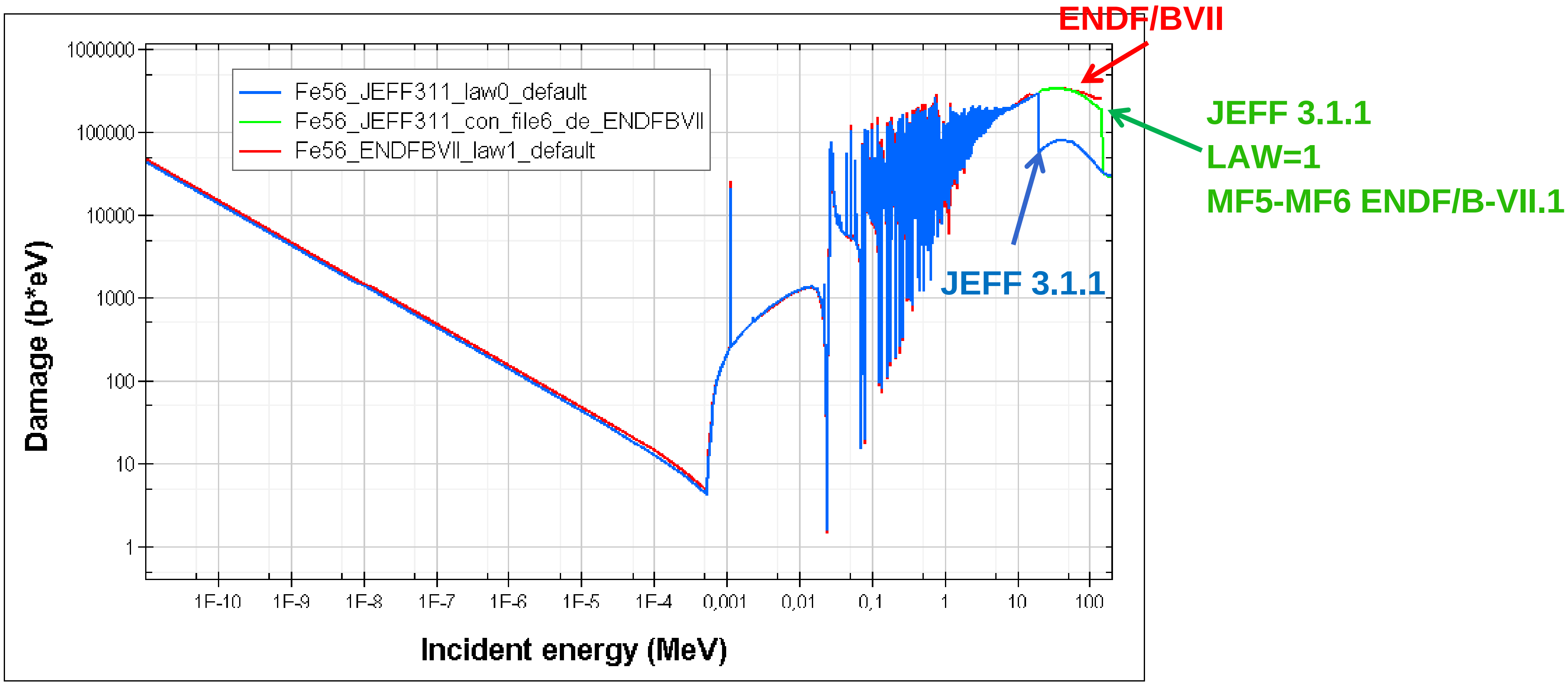


Figure. A comparison of Damage Energy Cross Section for Fe56. Updated JEFF-3.1.1 with MT5 and MT6 taken from ENDF/B-VII.1

Task 4.1 : What materials?

- Isotopes to be processed: (**structural materials**): Al, Ti, V, Cr, Fe, Ni, Cu and Zr

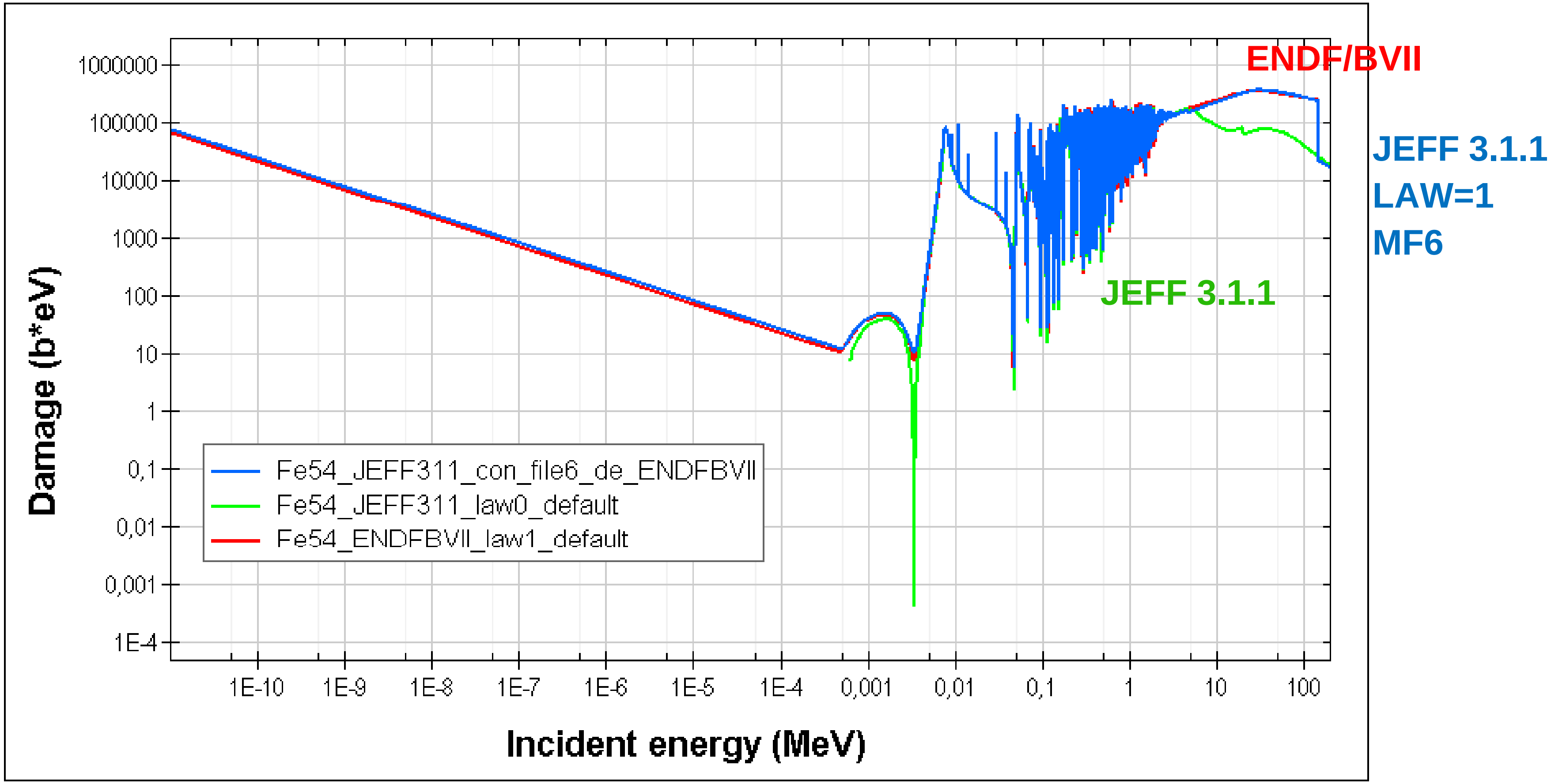
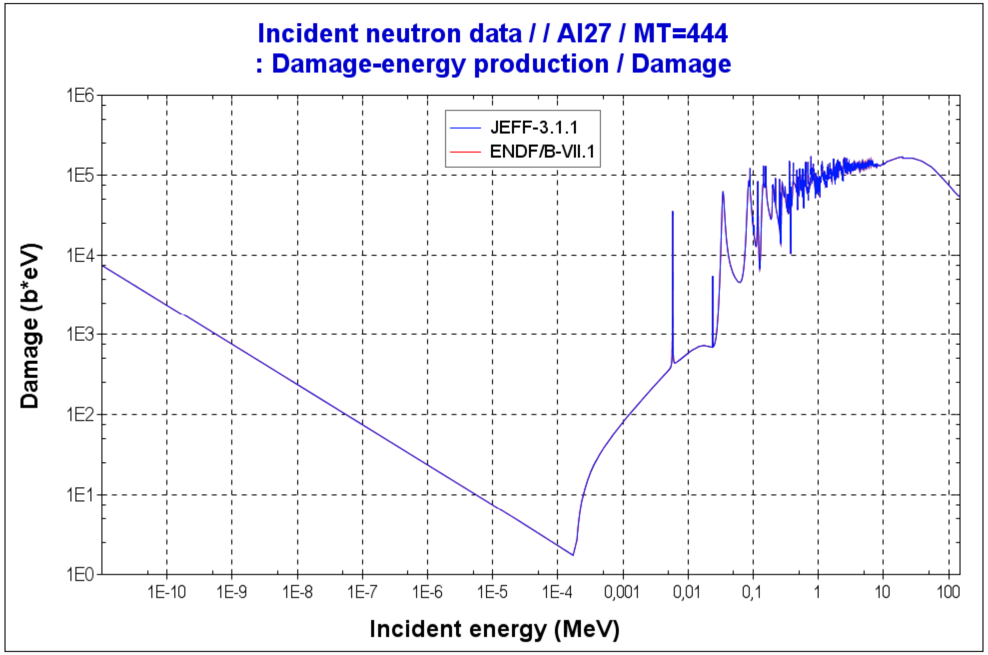


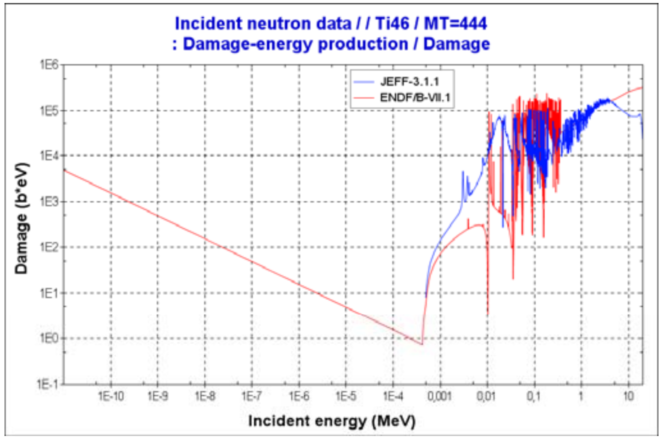
Figure. A comparison of Damage Energy Cross Section for Fe54.
Updated JEFF-3.1.1 with MT5 and MT6 taken from ENDF/B-VII.1

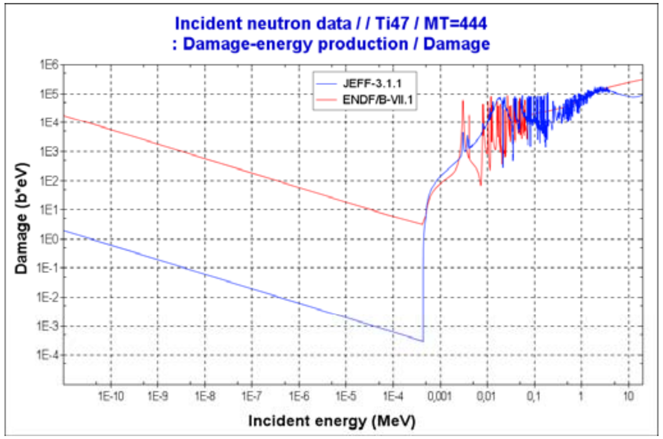
- $Ni^{58,59,60}$, Cr, V, Ti and Zr: JEFF 3.1.1 does not include information (MT3) above 20 MeV!!!

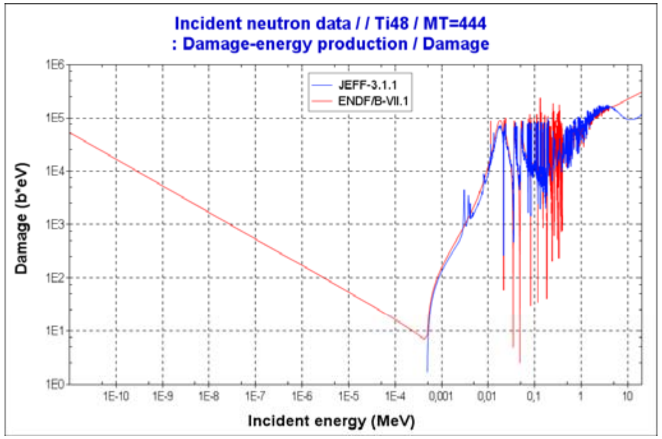
Task 4.1 : Alumnium

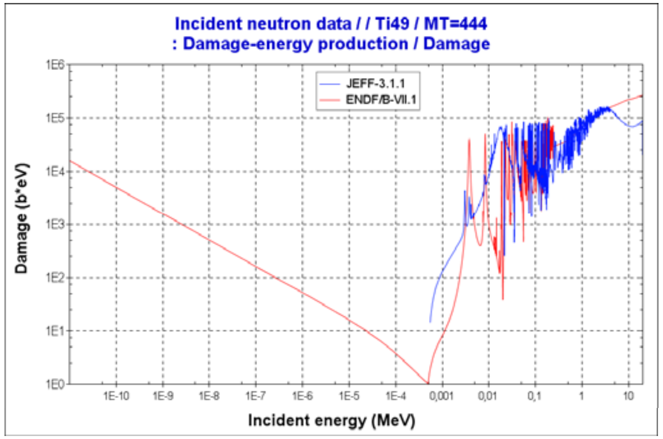


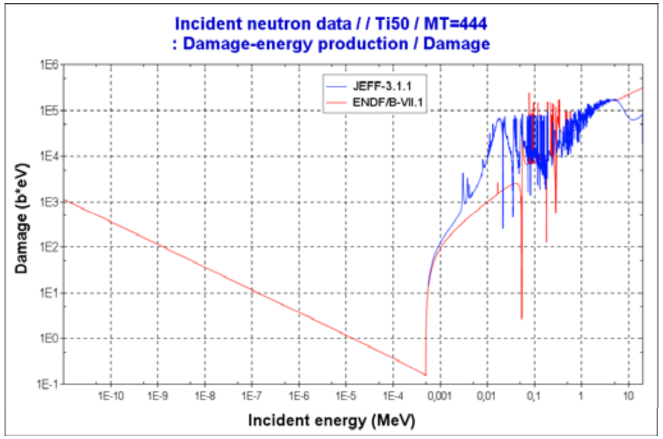
Task 4.1 : Titanium



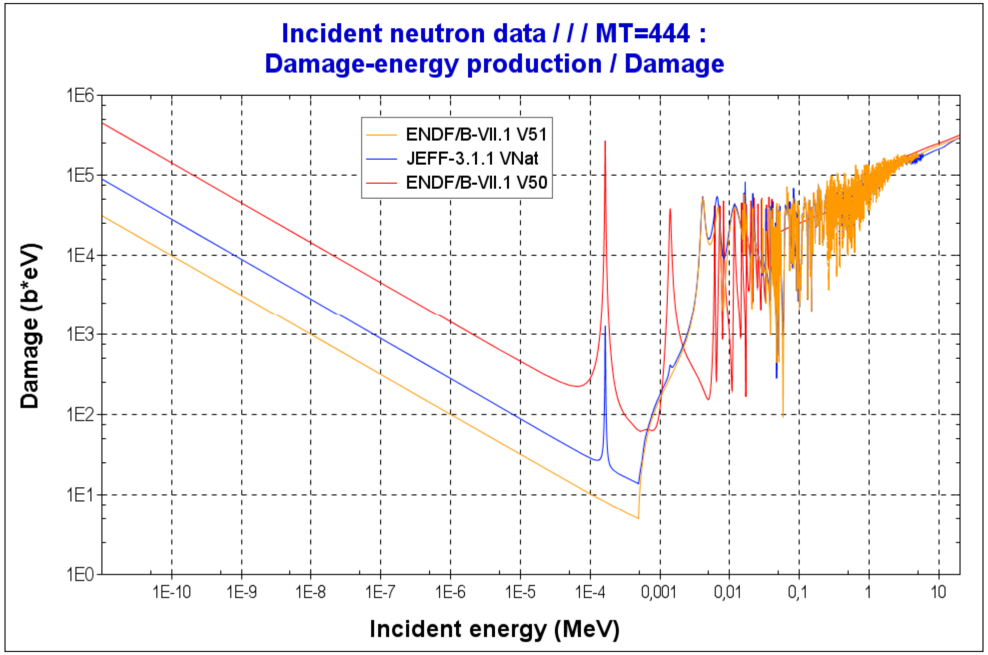




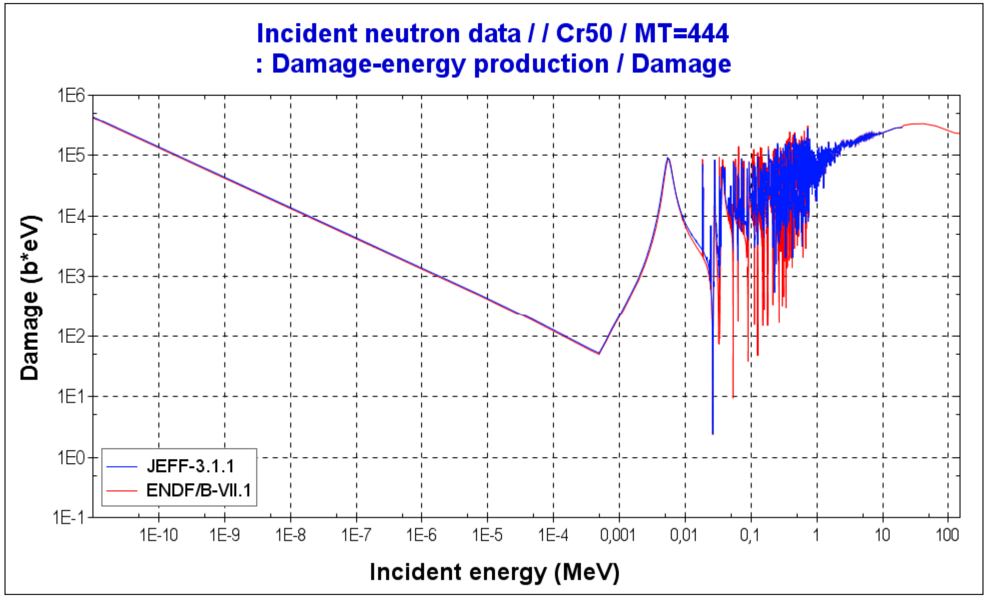


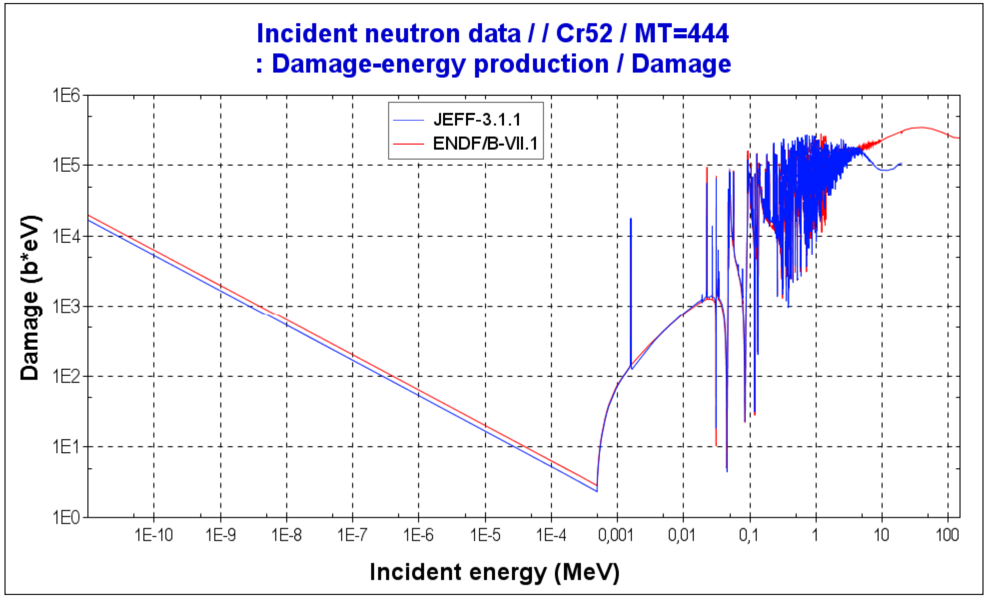


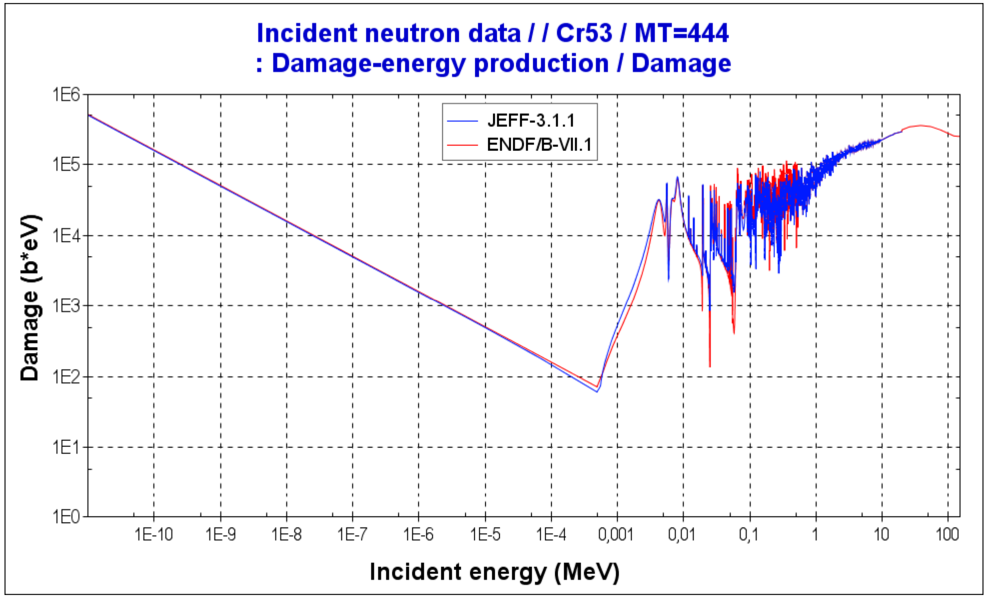
Task 4.1 : Vanadium

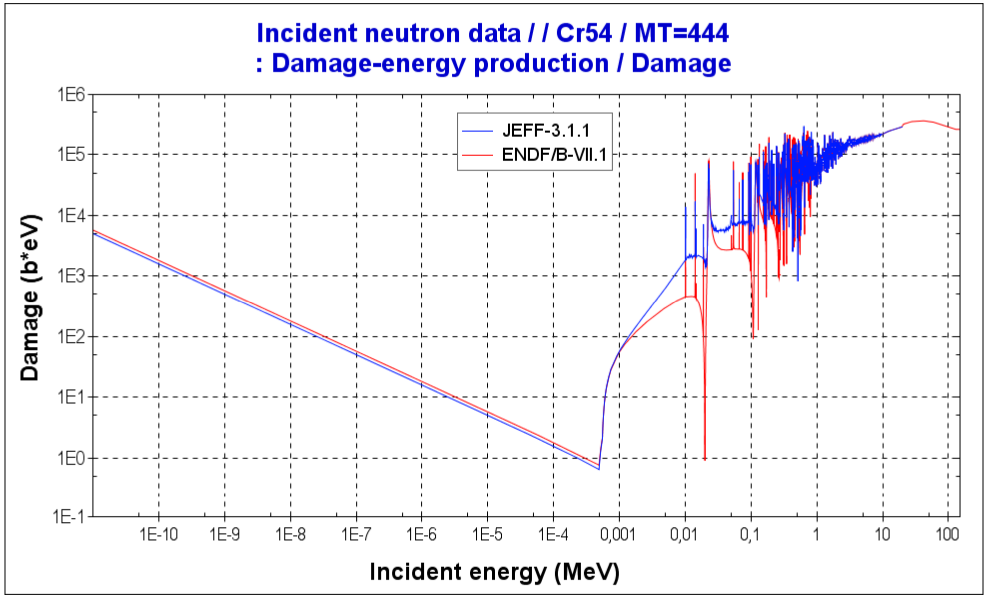


Task 4.1 : Chromium

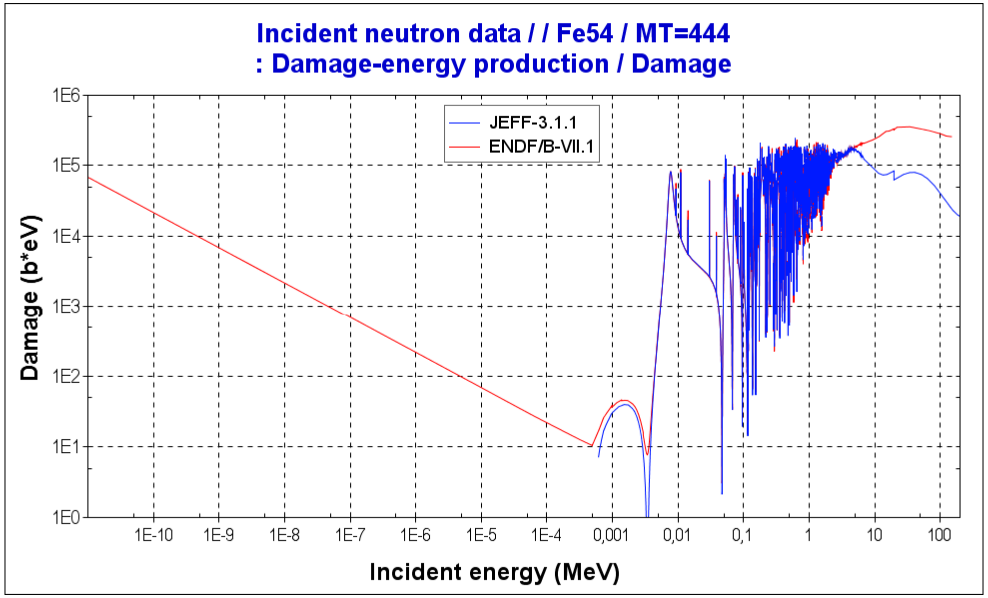


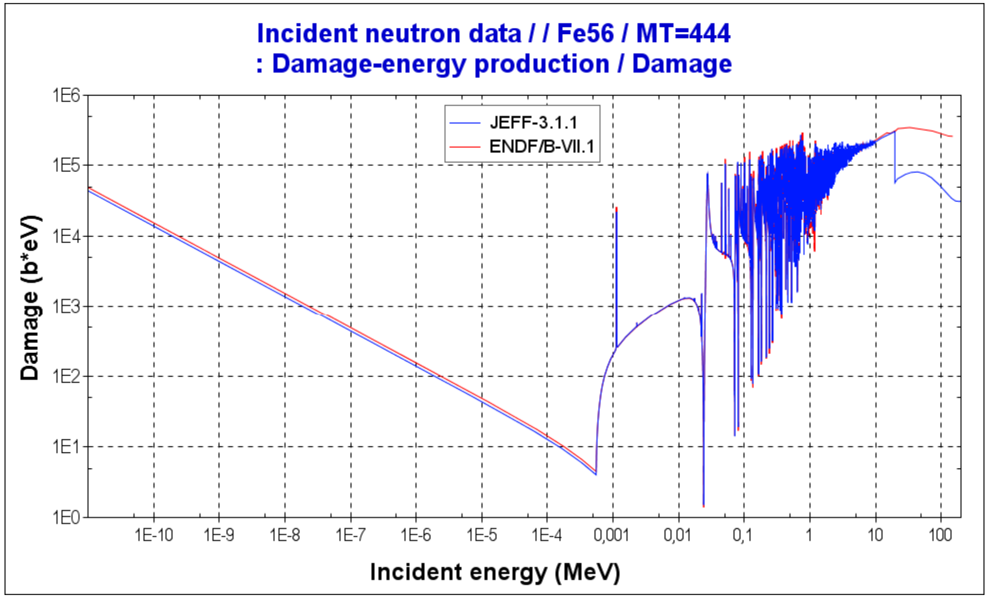






Task 4.1 : Iron


Incident neutron data / / Fe54 / MT=444
: Damage-energy production / Damage
JEFF-3.1.1
ENDF/B-VII.1
Damage (b*eV)
Incident energy (MeV)
1E0
1E1
1E2
1E3
1E4
1E5
1E6
1E-10
1E-9
1E-8
1E-7
1E-6
1E-5
1E-4
0,001
0,01
0,1
1
10
100


Incident neutron data / / Fe56 / MT=444
: Damage-energy production / Damage
JEFF-3.1.1
ENDF/B-VII.1
Damage (b*eV)
Incident energy (MeV)
1E0
1E1
1E2
1E3
1E4
1E5
1E6
1E-10
1E-9
1E-8
1E-7
1E-6
1E-5
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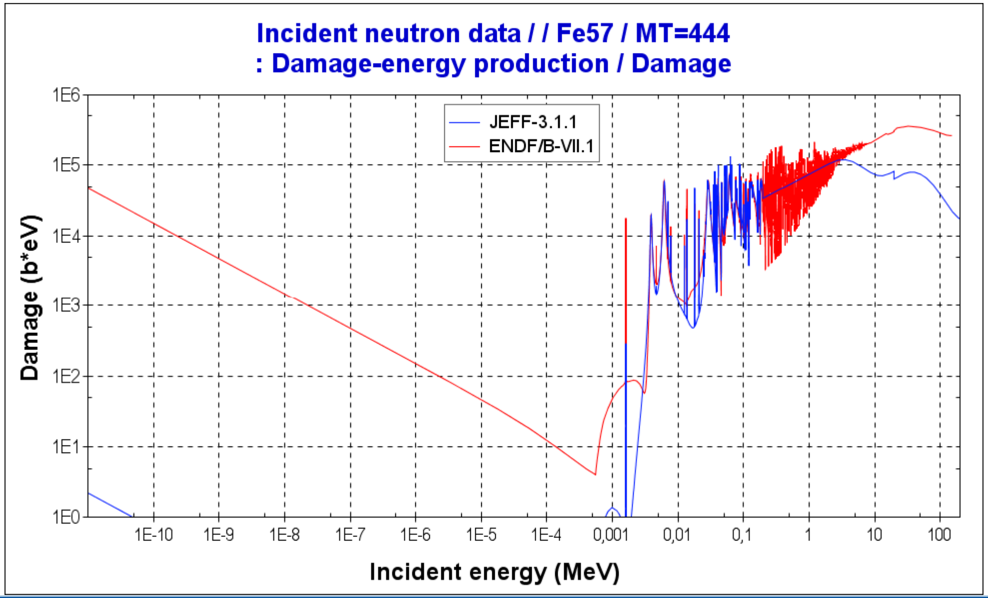
0,001
0,01
0,1
1
10
100


Incident neutron data / / Fe57 / MT=444
: Damage-energy production / Damage
JEFF-3.1.1
ENDF/B-VII.1
Damage (b*eV)
Incident energy (MeV)
1E0
1E1
1E2
1E3
1E4
1E5
1E6
1E-10
1E-9
1E-8
1E-7
1E-6
1E-5
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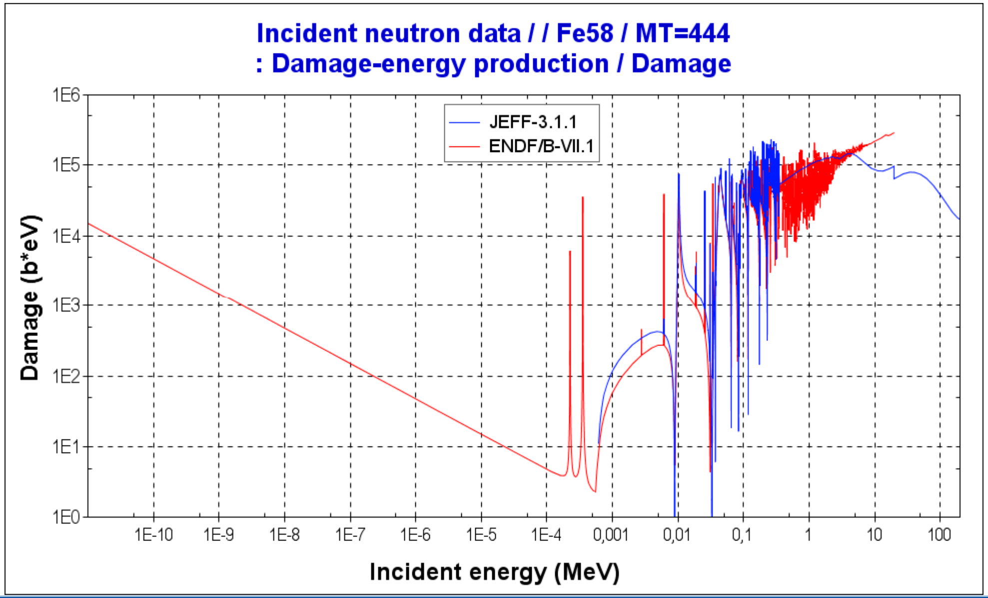
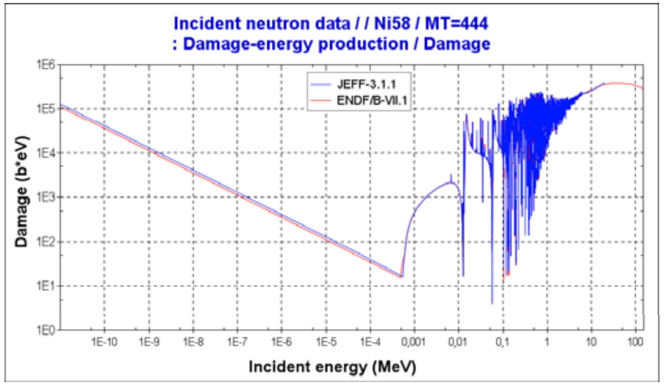
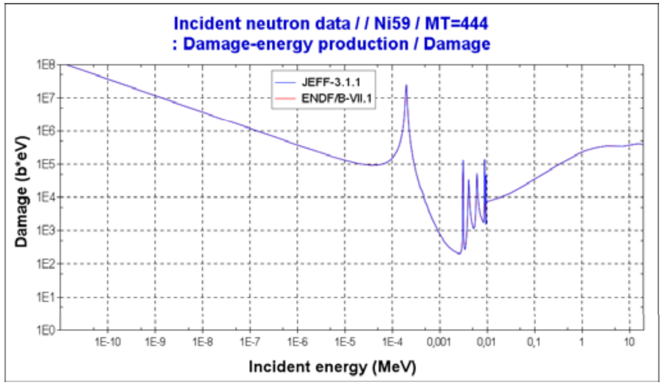
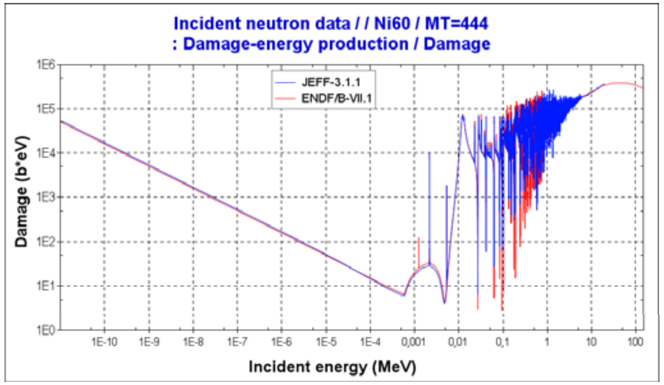
0,01
0,1
1
10
100

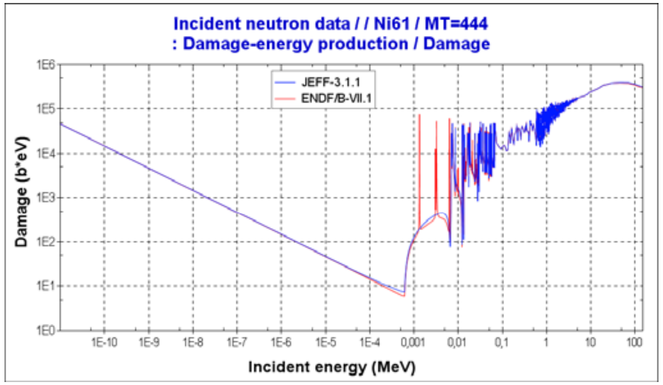

Incident neutron data / / Fe58 / MT=444
: Damage-energy production / Damage
JEFF-3.1.1
ENDF/B-VII.1
Damage (b*eV)
Incident energy (MeV)
1E0
1E1
1E2
1E3
1E4
1E5
1E6
1E-10
1E-9
1E-8
1E-7
1E-6
1E-5
1E-4
0,001
0,01
0,1
1
10
100

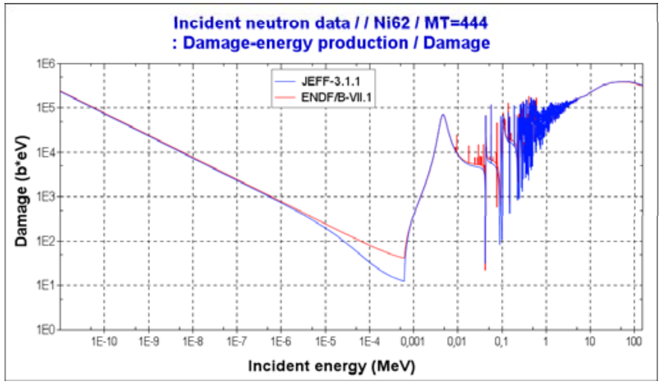
Task 4.1 : Nickel

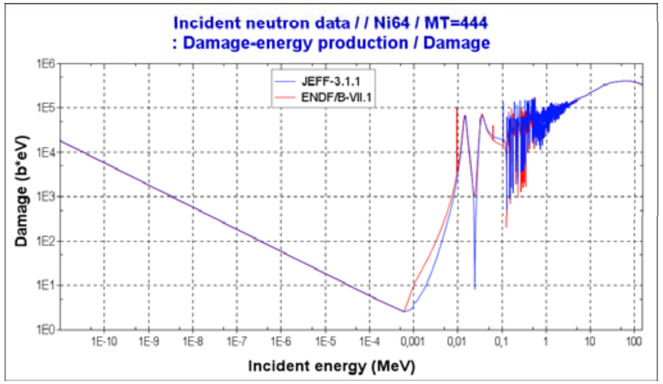




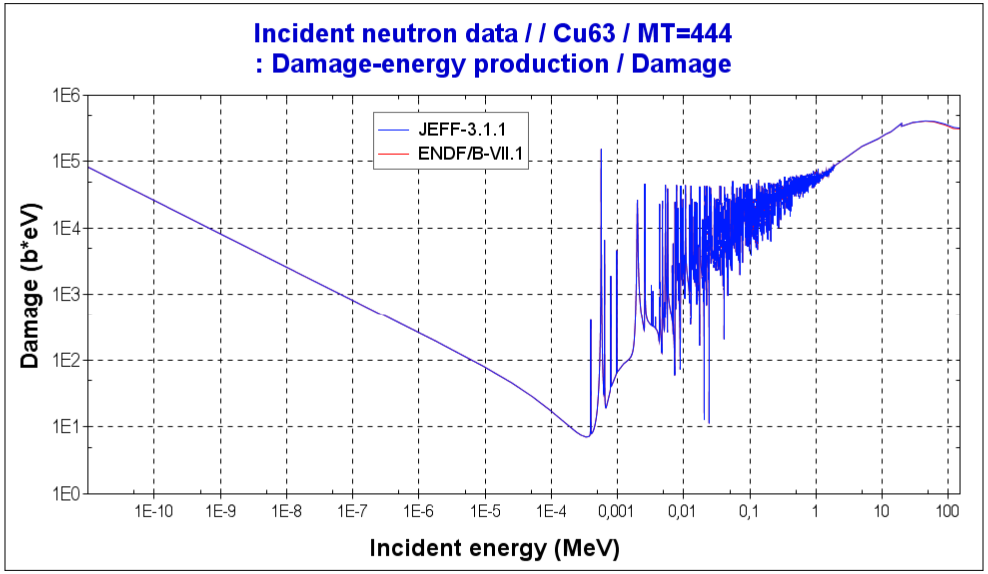


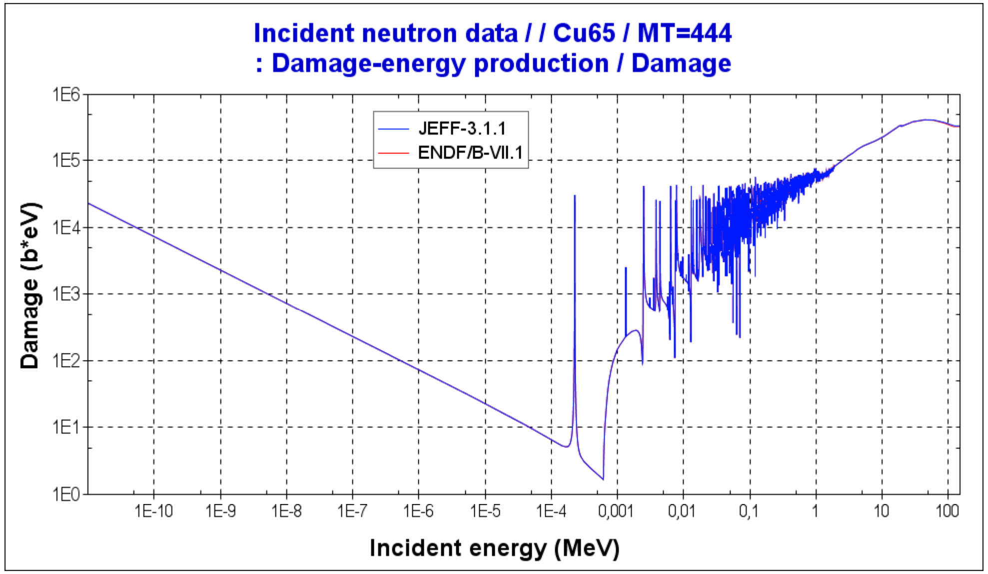




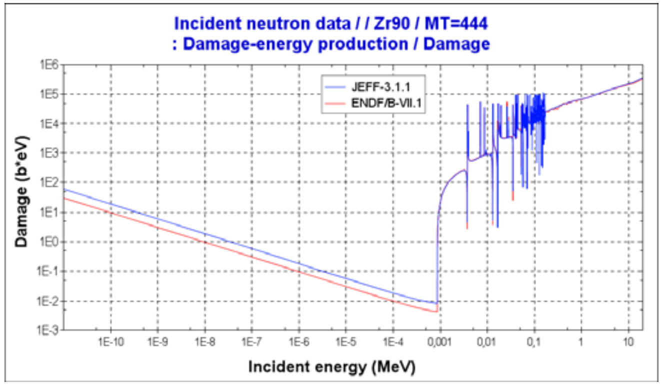


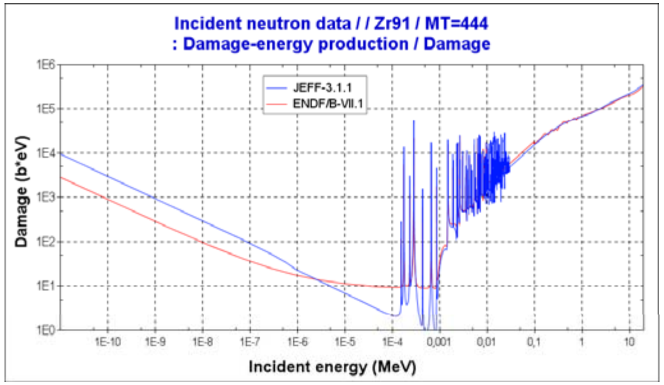
Task 4.1 : Copper

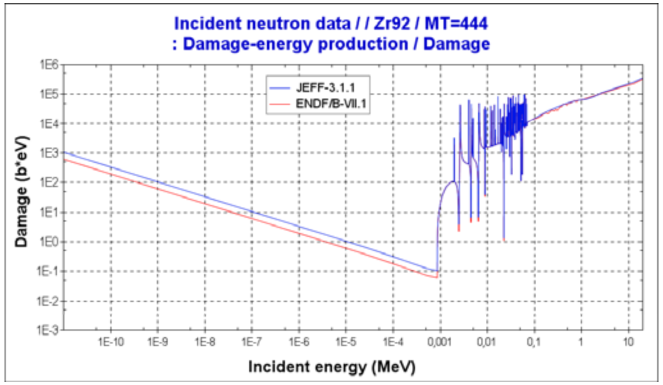


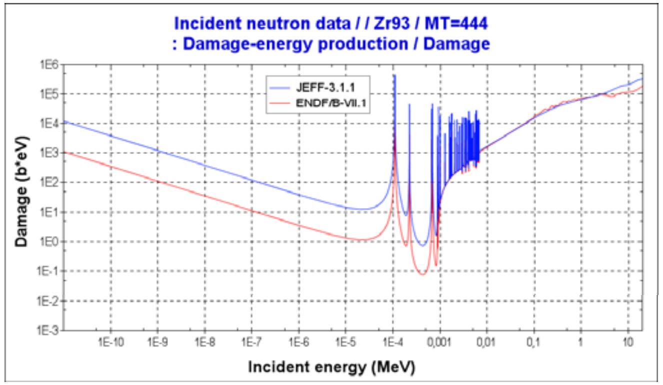


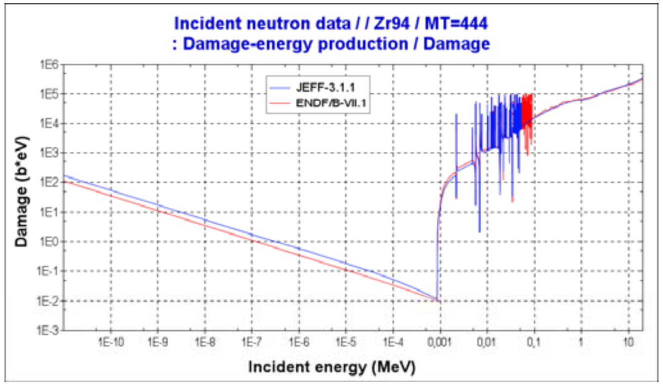
Task 4.1 : Zirconium

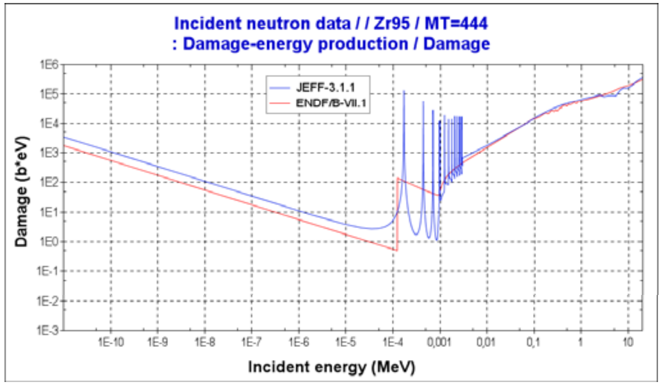


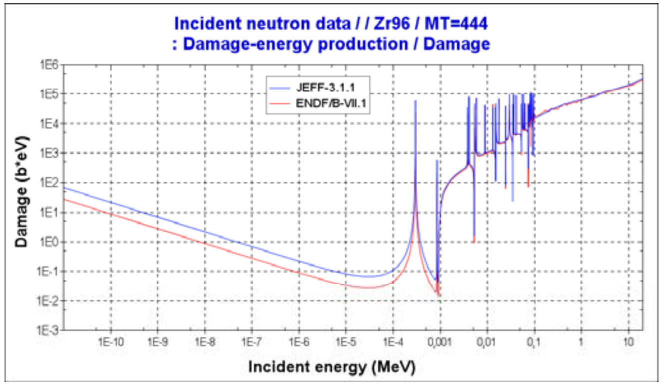












Task 4.1 : New Methodology…

- Neutron and proton induced displacement cross-sections were calculated for the main components of stainless steels using the binary collision approximation model (BCA) and results of molecular dynamics simulations (MD).
- NJOY uses of rough approximations for the calculations of the number of radiation defects based e. g. on the NRT model

$$\nu(T_i) = \eta N_{NRT}$$

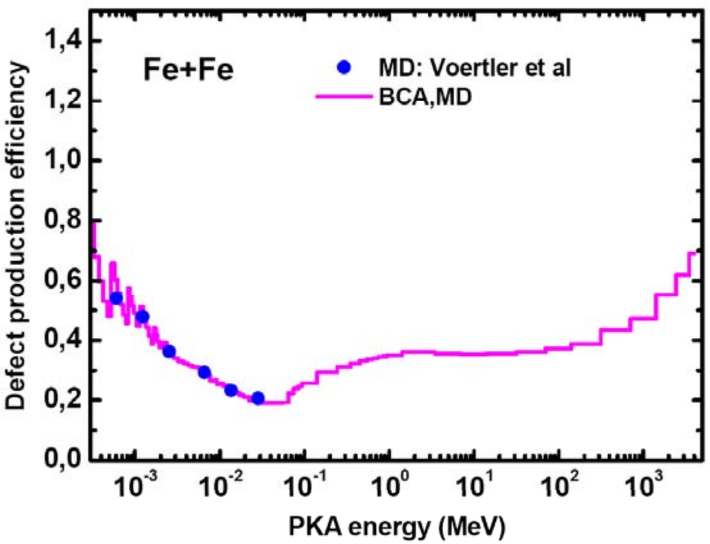


Figure: The efficiency of the defect production for the Fe-Fe irradiation obtained using the combined BCA,MD method and results of the MD simulation.

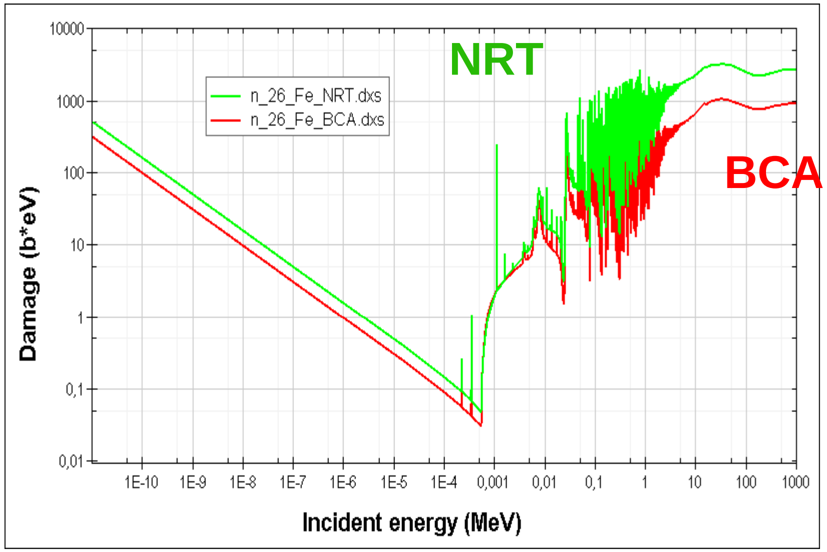


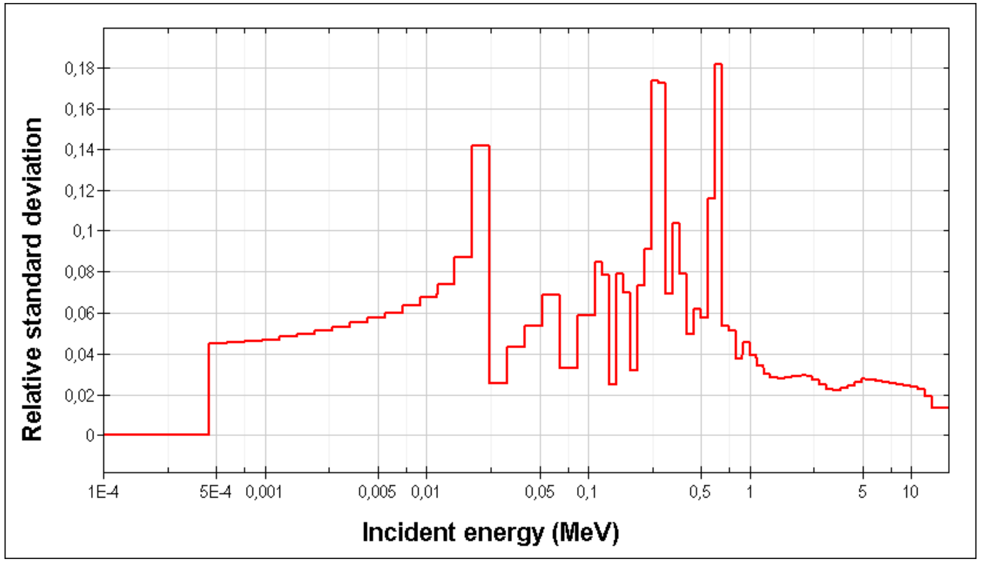
Figure: The displacement cross-section for neutron irradiation of iron obtained using BCA,MD approach and the NRT model.

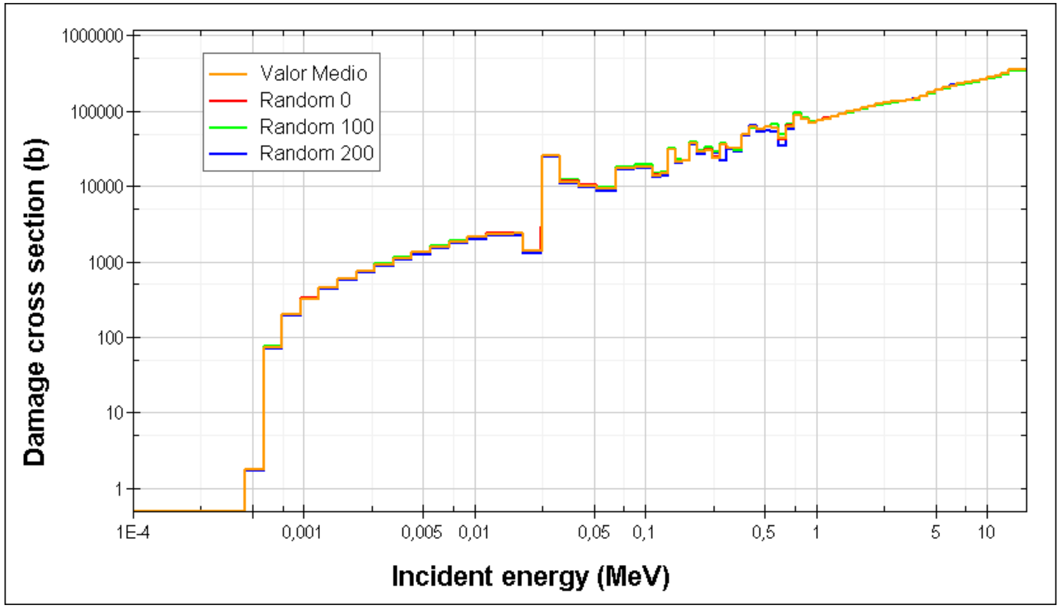
Ref. A.Yu. Konobeyev et al. "Displacement cross section files for structural materials irradiated with neutrons and protons", 2011

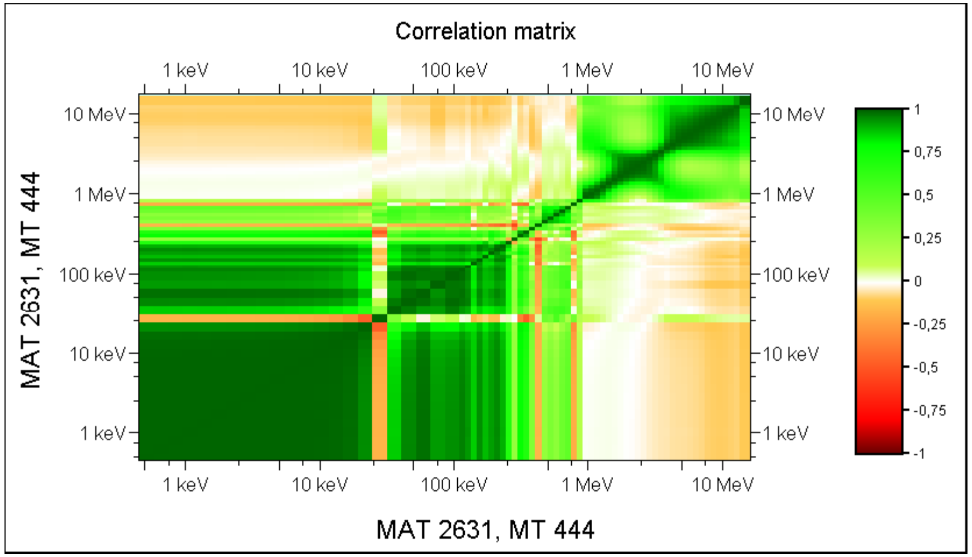
Task 4.1 : What about uncertainties?

Based on Total Monte Carlo methodology

- TENDL2011: 380 ENDF files
- Processing with NJOY/GROUPR







Task 6.2 : Background

Task 6.2 : Postprocessing of photonuclear libraries (**by CCFE**) and thermal scattering tables (**by UPM**) at the backend of the calculational system (CCFE/UPM)

- Revision of photonuclear/thermal scattering tables **(12 months)**
  - Comparison between: JEFF-3.1.1, ENDF/B-VII.1,…
- Processing with NJOY in multigroups and ACE format and testing with MCNPX code system (**12 months**)
- Release recommended produced Photonuclear/STL data library (**2 months**)

Photonuclear libraries before IAEA (2000)

Library	BOFOD-99	CNDC	JENDL	KAERI	LANL
Energy	< 20 MeV	< 30 MeV	< 140 MeV	7 – 140 MeV	< 150 MeV
Materials	70	24	51	143	10
Data	XS, α-E	XS, spec.	XS, spec.	XS indiv.	XS, spec.
Evaluation Methods	Exp. + Theor.	Exp. + Theor.	Exp. + Theor.	Exp. + Theor.	Exp. + Theor. [1]
Format	ENDF-6	ENDF-6	ENDF-6	ENDF-6	ENDF-6
Others	Be-Ta^{181} < 70 MeV	AUTOOPT, DREAM, GUNF & GLUNF	MCPHOTO, ALICE-F	GUNF & GNASH	

IAEA Photonuclear Library(2000)

Folder	CONTENS
Recommended	**IAEA Library. 164 isotopes selected from Other libraries**
Other Libraries	Libraries considered to build IAEA library
Other Files. BOFOD	27+36+9 materials: 9 selected
Other Files. CNDC	24 materials: 12 selected
Other Files. EPNDL	26 materials
Other Files. JENDL	18 materials: 10 selected
Other Files. KAERI	143 materials: 124 selected
Other Files. LANL	12 materials: 9 selected

Recent Photonuclear Libraries

Libraries	IAEA	JENDL/PD-2004	ENDF/B-VII.1	TENDL-2009 TENDL-2011
Energy	< 140 MeV	< 140 MeV	< 150 MeV *20-30 MeV	200 MeV
Materials	164	68	163	^{6}Li – ^{281}Ds
Evaluation Methods	GNASH + statistic	Better (γ,abs) Exp Data	IAEA Revision Exp. Bremsstr.	TALYS
Others		He, Li, B, F, P, Hg y Gd	Actinides	Isomeric States

Task 6.2 : A comparison …

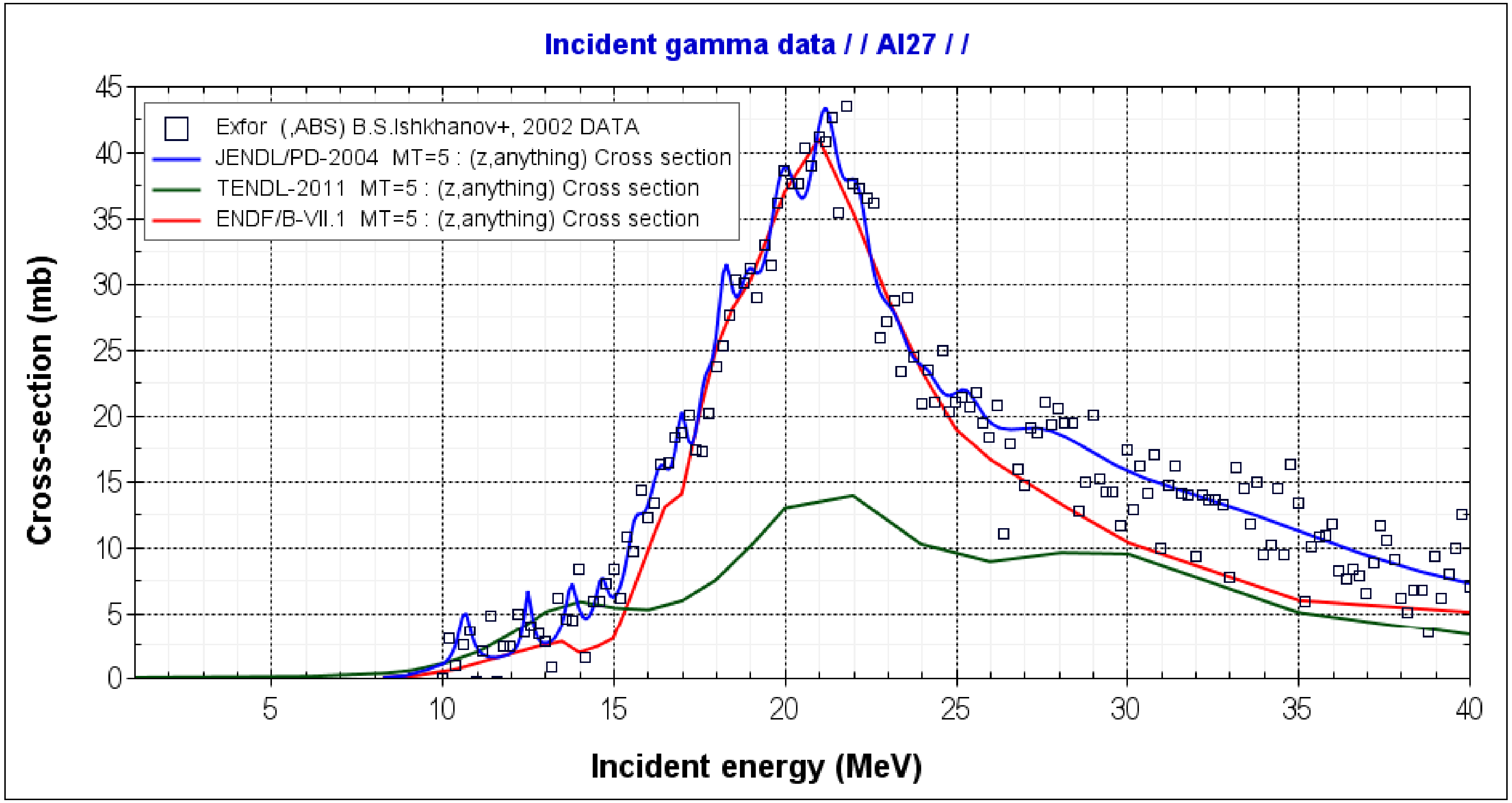


Figure. A comparison of total gamma cross section for Al27. JEFF-3.1.1, ENDF/B_VII.1 and JENDL-PD. Exfor Data: Ishkhanov 2002

Exfor data: Moscow State Uiversity. Nuclear Physics Intitute. Ishkhanov *et al.* 2002
Source: Quasi-monoenergetic photons, Annihilation radiation.

Task 6.2 : Processing with NJOY…

```
moder / Extract/convert
photonuclear data
1 41
'26-Fe-54 from ENDF/B-VII'/
40 2625
0/
moder / Extract/convert
photonuclear data
1 42
'26-Fe-54 from ENDF/B-VII'/
40 2625
0/
acer / Prepare ACE files
41 42 0 27 28
5/
'26-Fe-54 photo-nuclear'/
2625/
acer / Check ACE files
0 27 0 29 30
7 1 1 -1/
/
stop
```

Figure. NJOY Input to process Photonuclear Evaluated Files in ACE format

Task 6.2 : Application with MCNPX

Material	Electron beam	Neutron Yield per 10^6 Electrons					
Target	**Energy**	**Data Exp. B&G ****	**COG***	**MCNPX IAEA***	**MCNPX ENDF/B-VII.1 *This Work***	**MCNPX JENDL PD-2004 *This Work***	**MCNPX TENDL-2011 *This Work***
Aluminium	22.2 MeV	*46 ± 7*	*37 ± 1*	*35*	**37**	**37**	**23**
Aluminium	28.3 MeV	*210 ± 32*	*162 ± 1*	*158*	**170**	**170**	**130**
Aluminium	34.3 MeV	*430 ± 65*	*332 ± 2*	*329*	**330**	**330**	**250**

***Ref.** Photonuclear Benchmarks with a Comparison of COG and MCNPX. David P. Heinrichs and Edward M. Lent. Cross Section Evaluation Working Group (CSEWG) at the Meeting held at Brookhaven National Laboratory, November 4 - 6, 2003.

****Experiment**: W. C. Barber and W. D. George, “Neutron Yields from Targets Bombarded by Electrons”, Physical Review: 116 (6) 1551 – 1559, December 15, 1959

Processing of all Thermal Scattering Libraries in multigroups and ACE format using NJOY.

- Introduction to Thermal Scattering Libraries
- TSL in ENDF-6 format
- State of the Art
- Processing with NJOY
- Graphics

Importance of Thermal Scattering

Low energy neutrons have high associated wavelengths, similar to the size of molecules of crystalline lattices.

It can exchange energy with materials by modifying:

- The speed of the molecule
- The rotation
- The vibration

Types of Thermal Scattering

- **Inelastic**: Important for all materials and described by the scattering law $S(\alpha,\beta)$
- **Incoherent elastic**: Important for hydrogenous solids such as HZr
- **Coherent elastic**: Important for crystalline solids like Graphite.

Information in ENDF-6 format

INELASTIC SCATTERING: File 7, Section 4.

- The scattering law S(α,β) is tabulated.
- For high incident energies, α and/or β values might not be included.
- In these cases, the short-collision-time approximation has to be used, using additional data contained in ENDF-6 format.

ENDF-6 format

[MAT, 7, 4 / ZA, AWR, 0, LAT, LASYM, 0]HEAD
[MAT, 7, 4 / 0.0, 0.0, LLN, 0, NI, NS/B(N)] LIST
[MAT, 7, 4 / 0.0, 0.0, 0, 0, NR, NB/βint] TAB2
[MAT, 7, 4 / T0, β1, LT, 0, NR, NP/ αint / S(α, β1,T0)] TAB1
[MAT, 7, 4 / T1, β1, LI, 0, NP, 0/ S(α, β1, T1)] LIST

<continue with LIST records for T2,T3,...TLT+1>

[MAT, 7, 4 / T0, β2, LT, 0, NR, NP/ αint / S(α,β2,T0)] TAB1

<continue with TAB1 and LIST records for remaining values of β and T >

[MAT, 7, 4 / 0.0, 0.0, 0, 0, NR, NT/ Tint / Teff0(T)] TAB1

[MAT, 7, 0 / 0.0, 0.0, 0, 0, 0, 0] SEND

$$\frac{d^2\sigma}{d\Omega dE'} = \sum_{n=0}^{NS} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}}\, e^{-\beta/2} S_n(\alpha,\beta,T)$$

$$S^{SCT} = \frac{\exp\left[-\frac{(\alpha-|\beta|)^2 T}{4\alpha T_{eff}(T)} - \frac{|\beta|}{2}\right]}{\sqrt{4\pi\alpha \frac{T_{eff}(T)}{T}}}$$

Information in ENDF-6 format

COHERENT ELASTIC SCATTERING: File 7, Section 2.

The quantity given in the libraries is $S(E,T) = \sum_{i=1}^{E_i<E} s_i(T)$

[MAT, 7, 2/ ZA, AWR, LTHR, 0, 0, 0] HEAD LTHR=1
[MAT, 7, 2/ T0, 0.0, LT, 0, NR, NP/ Eint / S(E,T0)] TAB1
[MAT, 7, 2/ T1, 0.0, LI, 0, NP, 0/ S(Ei,T1)] LIST

<repeat LIST for T2, T3, ...TLT>

[MAT, 7, 0/0.0, 0.0, 0, 0, 0, 0] SEND

$$\frac{d^2\sigma}{dE'd\Omega} = \frac{1}{E}\sum_{i=1}^{E_i<E} s_i(T)\delta(\mu-\mu_i)\delta(E-E')/2\pi$$

INCOHERENT ELASTIC SCATTERING: File 7, Section 2.

The information given is W', the DebyeWaller integral divided by the atomic mass (eV^{-1})

[MAT, 7, 2/ ZA, AWR, LTHR, 0, 0, 0]HEAD (LTHR=2)
[MAT, 7, 2/ SB, 0.0, 0, 0, NR, NP/ Tint / W'(T)]TAB1
[MAT, 7, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND

$$\frac{d^2\sigma}{dE'd\Omega} = \frac{\sigma_b}{4\pi} e^{-2EW'(T)(1-\mu)}\delta(E-E')$$

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State of the Art: Temperatures

Isotope	Compound	ENDF/B-VI.8 and JENDL-4.0. 20 materials	ENDF/B-VII.0 and ENDF/B-VII.1 20 and 21 mats.	INDL-TSL 11 materials	JEFF 3.1.X 9 materials
H	H2O Problems processing all libraries	296, 350, 400, 450, 500, 600, 800, 1000	293.6, 350, 400, 450, 500, 550, 600, 650, 800	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, 1000	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, 1000
H	Para-H	20	20	14, 16, 20.38	-
H	Ortho-H	20	20	14, 16, 20.38	-
H	HZr	296, 400, 500, 600, 700, 800, 1000, 1200 Without secondary scatterer.	296, 400, 500, 600, 700, 800, 1000, 1200 Without secondary scatterer.	293.6, 400, 500, 600, 700, 800, 1000, 1200 With secondary scatterer.	293.6, 400, 500, 600, 700, 800, 1000, 1200 With secondary scatterer.
H	CaH2	-	-	-	296, 400, 500, 600, 700, 800, 1000, 1200
H	TiH2	-	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-

State of the Art: Temperatures

Isotope	Compound	ENDF/B-VI.8 and JENDL-4.0	ENDF/B-VII.0 and ENDF/B-VII.1	INDL-TSL	JEFF 3.1.X
H	YH2	-	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-
H	CeH2	-	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-
H	l-CH4	100	100	-	-
H	S-CH4	22	22	-	-
H	CH2	296, 350	296, 350	-	293.6, 350
H	C6H6	296, 350, 400, 450, 500, 600, 800, 1000	296, 350, 400, 450, 500, 600, 800, 1000	-	-
D	D2O	296, 350, 400, 450, 500, 600, 800, 1000	293.6, 350, 400, 450, 500, 550, 600, 650	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 643.9,	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 643.9,
D	Para-D	19	19	19, 23.65	-
D	Ortho-D	19	19	19, 23.65	-

State of the Art: Temperatures

Isotope	Compound	ENDF/B-VI.8 and JENDL-4.0	ENDF/B-VII.0 and ENDF/B-VII.1	INDL-TSL	JEFF 3.1.X
C	Graphite	296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000	296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000	293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, 3000	293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, 3000
Be	Be metal	296, 400, 500, 600, 700, 800, 1000, 1200	296, 400, 500, 600, 700, 800, 1000, 1200	-	293.6, 400, 500, 600, 700, 800, 1000, 1200. Problems while processing. Fixed file available in JEFF-B
Be	BeO	296, 400, 500, 600, 700, 800, 1000, 1200 With secondary scatterer	293.6, 400, 500, 600, 700, 800, 1000, 1200 Without secondary scatterer	-	-
U	UO2	-	296, 400, 500, 600, 700, 800, 1000, 1200	-	-
O	UO2	-	296, 400, 500, 600, 700, 800, 1000, 1200	-	-
O	BeO	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-	-

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State of the Art: Temperatures

Isotope	Compound	ENDF/B-VI.8 and JENDL-4.0	ENDF/B-VII.0 and ENDF/B-VII.1	INDL-TSL	JEFF 3.1.X
Zr	HZr	296, 400, 500, 600, 700, 800, 1000, 1200	296, 400, 500, 600, 700, 800, 1000, 1200	-	-
Ca	CaH2	-	-	-	296, 400, 500, 600, 700, 800, 1000, 1200
Si	SiO2	-	293.6, 350, 400, 500, 800, 1000, 1200 Only in ENDF/B-VII.1	-	-
Mg	Mg	-	-	-	20, 100, 296, 773
Al	Al	-	20, 80, 293.6, 400, 600, 800	-	-
Fe	Fe	-	20, 80, 293.6, 400, 600, 800	-	-

Table . Information on the JEFF-3.1.2 Thermal Scattering ACE library at different temperatures

Temp (K)	Hydrogen bound in water	Hydrogen bound in polyethylene	Hydrogen bound in ZrH	Graphite	D bound in D2O	Be	Ca bound in CaH2	H bound in CaH2	Mg24
20									mg00.32t
100									mg01.32t
293.6	lw00.32t	pol00.32t	hzr00.32t	gr00.32t	hw00.32t	be00.32t			
296							ca00.32t	hcah200.32t	mg02.32t
323	lw01.32t				hw01.32t				
350		pol01.32t							
373	lw02.32t				hw02.32t				
400			hzr01.32t	gr01.32t		be01.32t	ca01.32t	hcah201.32t	
423	lw03.32t				hw03.32t				
473	lw04.32t				hw04.32t				
500			hzr02.32t	gr02.32t		be02.32t	ca02.32t	hcah202.32t	
523	lw05.32t				hw05.32t				
573	lw06.32t				hw06.32t				
600			hzr03.32t	gr03.32t		be03.32t	ca03.32t	hcah203.32t	
623	lw07.32t								
643					hw07.32t				
647	lw08.32t								
700			hzr04.32t	gr04.32t		be04.32t	ca04.32t	hcah204.32t	
773									mg03.32t
800	lw09.32t		hzr05.32t	gr05.32t		be05.32t	ca05.32t	hcah205.32t	
1000	lw10.32t		hzr06.32t	gr06.32t		be06.32t	ca06.32t	hcah206.32t	
1200			hzr07.32t	gr07.32t		be07.32t	ca07.32t	hcah207.32t	
1600				gr08.32t					
2000				gr09.32t					
3000				gr10.32t					

Suff
(id suffix for zaid)

ENDF/B-VI.8: .68t
ENDF/B-VII.0: .70t
ENDF/B-VII.0: .71t
INDL-TSL: .20t

Libraries in ACE format

All the previous information has already been processed in ACE format using NJOY.

Figure. NJOY input to generate ACE Thermal Scattering library for C bound in Graphite at 293.6K

```
thermr / Add thermal scattering data (free gas)
0 23 62
0 600 12 1 1 1 1 221 1/
293.6
0.001 4.0
thermr / Add thermal scattering data (bound)
61 62 27
31 600 16 1 4 1 1 229 1/
293.6
0.001 4.0
acer / Prepare ACE files
21 27 0 28 29
2 0 1 .32/
'Graphi 293.6 K from (JEFF-3.1.2) NJOY99.364,  Dec2012'/
600 293.6 'gr00 ' /
6000 0 0 /
229 64 230 0 1 4.0 0/
acer / Check ACE files
0 28 0 71 81
7 1 1 -1/
/
```

Type of ACER run option	IOPT:	2 (THERMAL DATA)
Print control	IPRINT:	0 (MINIMUN)
ACE output type	NTYPE:	1
ID suffix for ZAID	SUFF:	.32
Material to be processed	MATD:	600
Temperature desired	NTEMPD:	293.6K
Thermal ZAID name	TNAME:	'gr00'
MT for thermal incoherent data*	MTI:	229
Number of bins for incoherent scattering+	NBINT:	64
MT for thermal elastic data*	MTE:	230
COHERENT/INCOHERENT ELASTIC	IELAS	0/1
Number of atom types in mixed moderator	NMIX:	1
Max. energy+	EMAX:	4.0 eV
Weight option	IWT:	0/1 VARIABLE/CONSTANT

* MTI and MTE values from Table 3 included in section XVII-22 (ACER module) in NJOY manual.
\+ Private communication, M.Mattes, IKE.

Libraries in ACE format

Table. Information of the JEFF-3.1.2 Thermal Scattering ACE library.

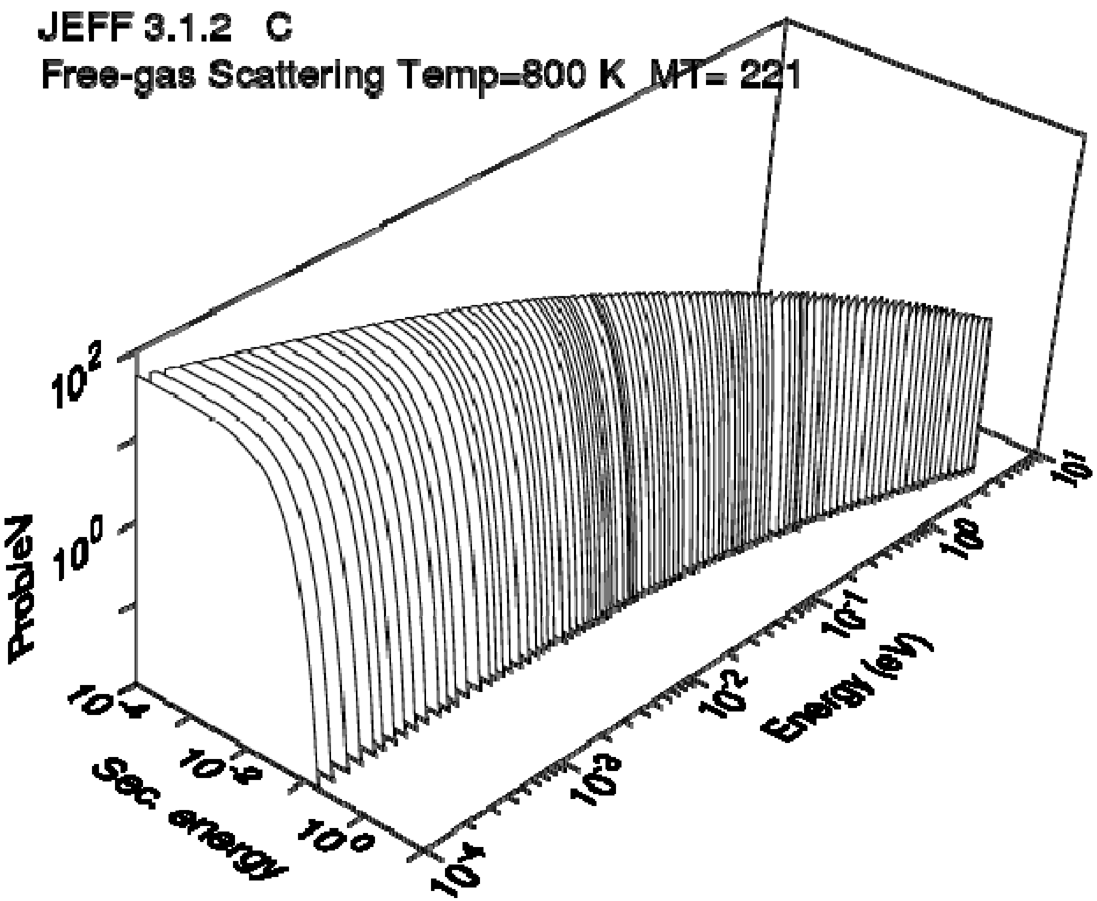
No.	Nuclide	ZAID	ACE filename	XSDIR filename
1	pol00.32t	Hydrogen bound in polyethylene	CH2-293.ace	CH2-293.dir
2	lw00.32t	Hydrogen bound in water	H2O-293.ace	H2O-293.dir
3	hzr00.32t	Hydrogen bound in ZrH	HZr-293.ace	HZr-293.dir
4	gr00.32t	Graphite	Gra-293.ace	Gra-293.dir
5	hw00.32t	D bound in D2O	D2O-293.ace	D2O-293.dir
6	be00.32t	Be	Be-293.ace	Be-293.dir
7	ca00.32t	Ca bound in CaH2	Ca(CaH2)-296.ace	Ca(CaH2)-296.dir
8	hcah200.32t	H bound in CaH2	H(CaH2)-296.ace	H(CaH2)-296.dir
9	mg00.32t	Mg-24	Mg24-20.ace	Mg24-20.dir

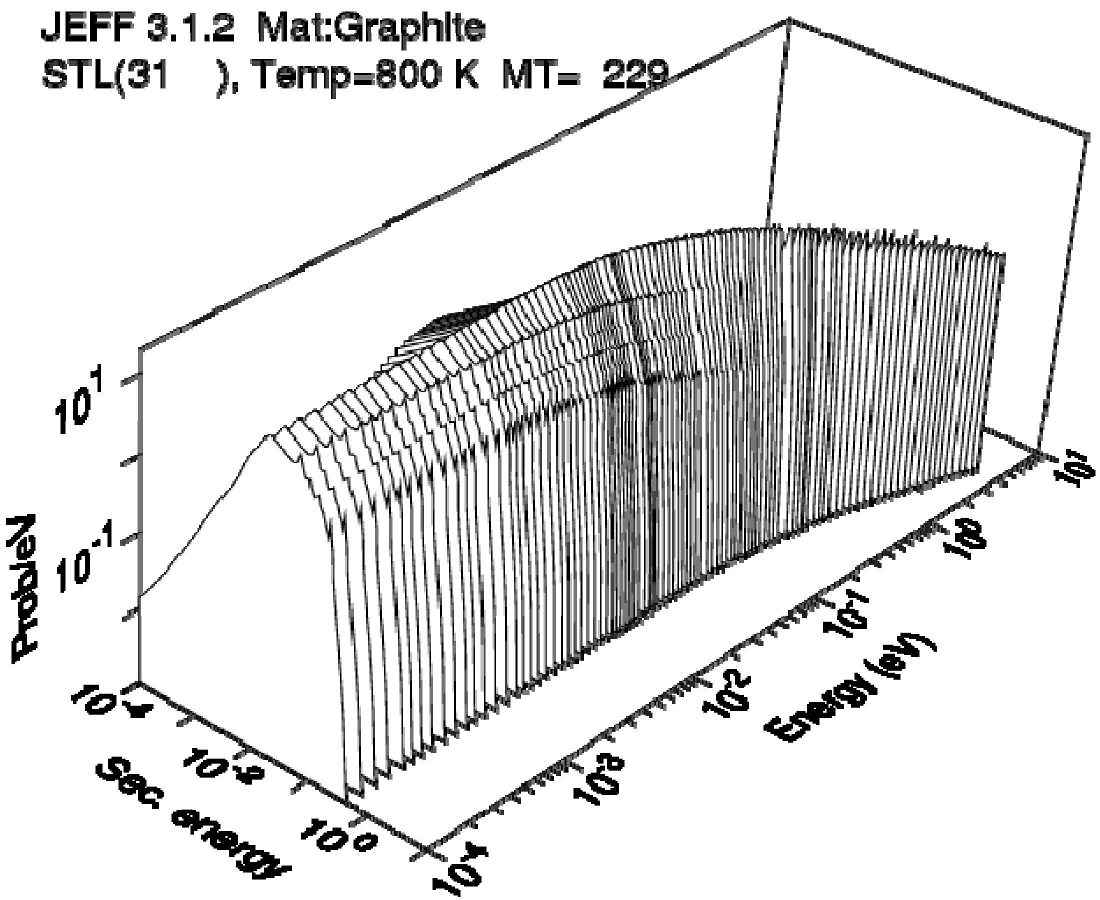
To take into account different temperatures in the STLs, the identification format will change according: “<mm><xx>.32t”, where <mm>=lw, pol, hzr, … is the associated identification to material, and <xx>=00,01,02,03, …, is the associated identification to temperature.

Graphics

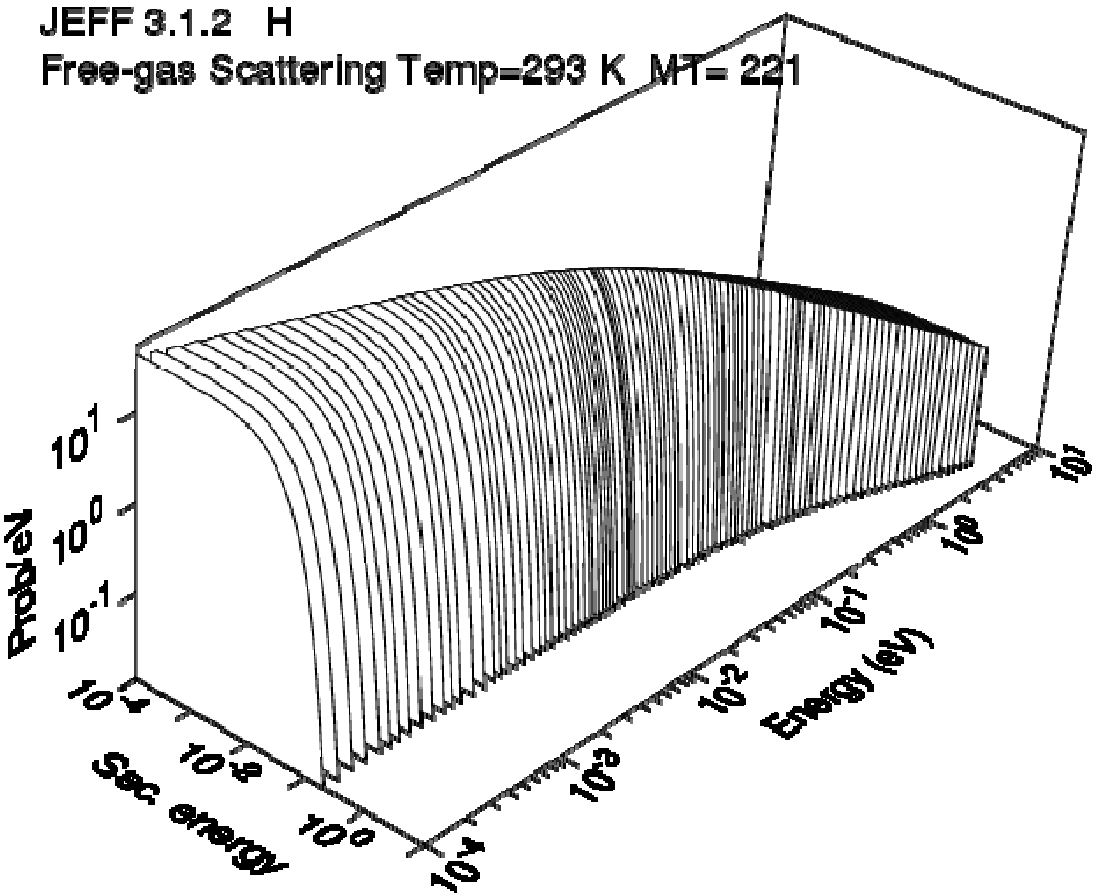
While processing, graphics for all materials have been generated for all available temperatures using the modules plotr and viewr of NJOY.

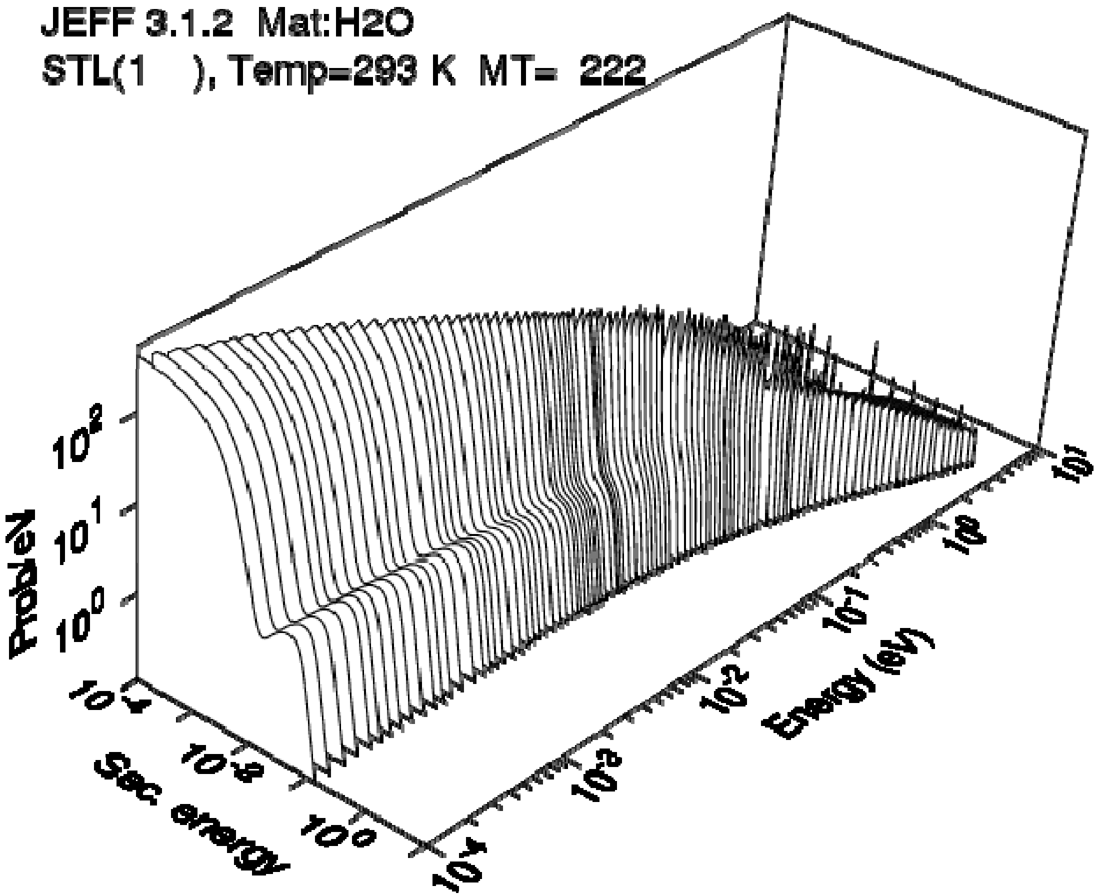
There are two kind of graphics: Free gas scattering and Bound scattering





Graphics


JEFF 3.1.2 H
Free-gas Scattering Temp=293 K MT= 221
ProbleN
Sec. energy
Energy (eV)


JEFF 3.1.2 Mat:H2O
STL(1), Temp=293 K MT= 222
ProbleN
Sec. energy
Energy (eV)

Future Actions

- Definition of a criticality/shielding Validation Suite for V&V with MNCP?
- Using LEAPR/NJOY module to generate S(α,β)
- Ref. *M. Mattes and J. Keinert, Thermal Neutron Scattering Data for the Moderator Materials H2O, D2O and ZrHx in ENDF-6 Format and as ACE Library for MCNP(X) Codes, indc-nds-0470, 2005*